# HIGH RESOLUTION MEASUREMENTS AND ELECTRONIC STRUCTURE CALCULATIONS OF A DIAZANAPHTHALENE

SÉBASTIEN GRUET[a], *AILES beamline, Synchrotron SOLEIL, Saint Aubin, France*; MANUEL GOUBET, *Laboratoire PhLAM, Université de Lille 1, Villeneuve de Ascq, France*; OLIVIER PIRALI, *Institut des Sciences Moléculaires d'Orsay, Université Paris-Sud, Orsay, France*.

Polycyclic Aromatic Hydrocarbons (PAHs) have long been suspected to be the carriers of so called Unidentified Infrared Bands (UIBs).[b] Most of the results published in the literature report rotationally unresolved spectra of pure carbon as well as heteroatom-containing PAHs species. To date for this class of molecules, the principal source of rotational informations is ruled by microwave (MW) spectroscopy [c] while high resolution measurements reporting rotational structure of the infrared (IR) vibrational bands are very scarce. Recently, some high resolution techniques provided interesting new results to rotationally resolve the IR and far-IR bands of these large carbonated molecules of astrophysical interest.[d] One of them is to use the bright synchrotron radiation as IR continuum source of a high resolution Fourier transform (FTIR) spectrometer. We report the very complementary analysis of the [1,6] naphthyridine (a N-bearing PAH) for which we recorded the microwave spectrum at the PhLAM laboratory (Lille) and the high resolution far-infrared spectrum on the AILES beamline at synchrotron facility SOLEIL. MW spectroscopy provided highly accurate rotational constants in the ground state to perform Ground State Combinations Differences (GSCD) allowing the analysis of the two most intense FT-FIR bands in the 50-900 $\mathrm{cm}^{-1}$ range. Moreover, during this presentation the negative value of the inertial defect in the GS of the molecule will be discussed.

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[a] Also at: Institut des Sciences Moléculaires d'Orsay, UMR 8214 CNRS-Université Paris Sud 91405 Orsay Cedex

[b] A. Leger, J. L. Puget, *Astron. Astrophys.* **137**, L5-L8 (1984); L. J. Allamandola et al. *Astrophys. J.* **290**, L25-L28 (1985).

[c] Z. Kisiel et al. *J. Mol. Spectrosc.* **217**, 115 (2003); S. Thorwirth et al. *Astrophys. J.* **662**, 1309 (2007); D. McNaughton et al. *J. Chem. Phys.* **124**, 154305 (2011).

[d] S. Albert et al. *Faraday Discuss.* **150**, 71-99 (2011); B. E. Brumfield et al. *Phys. Chem. Lett.* **3**, 1985-1988 (2012); O. Pirali et al. *Phys. Chem. Chem. Phys.* **15**, 10141 (2013).